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Shannon (Information) Measures of Symmetry for 1D and 2D Shapes and Patterns

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Abstract: In this paper, informational (Shannon) measures of symmetry are introduced and analyzed for patterns built of 1D and 2D shapes. The informational measure of symmetry $H_{sym}(G)$ characterizes the averaged uncertainty in the presence of symmetry elements from group G in a given pattern, whereas the Shannon-like measure of symmetry $\Omega_{sym}(G)$ quantifies the averaged uncertainty of the appearance of shapes possessing a total of n elements of symmetry belonging to group G in a given pattern. $H_{sym}(G_1) = \Omega_{sym}(G_1) = 0$ for the patterns built of irregular, non-symmetric shapes, where G_1 is the identity element of the symmetry group. Both informational measures of symmetry are intensive parameters of the pattern and do not depend on the number of shapes, their size, and the entire area of the pattern. They are also insensitive to the long-range order (translational symmetry) inherent for the pattern. Additionally, informational measures of symmetry of fractal patterns are addressed, the mixed patterns including curves and shapes are considered, the time evolution of Shannon measures of symmetry are examined, the close-packed and dispersed 2D patterns are analyzed, and an application of the suggested measures of symmetry for the analysis of the chemical reaction is demonstrated.

Keywords: informational measure of symmetry; 1D shapes; 2D shapes; fractal patterns; time evolution; symmetry; pattern

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1. Introduction

The notion of symmetry, which emerged from the Greek word συμμετρία meaning agreement in dimensions and arrangement, plays a crucial and instructive role in mathematics and natural sciences [1–5], generating conservation laws [6] and being crtitically important in materials science [7]; physics [2,5,6]; quantum theory [8]; quantum chemistry and spectroscopy [9]; and of course, crystallography [10,11]. Ideas, methods, and techniques arising from spatial symmetry are of fundamental importance in the philosophy and psychology of aesthetics [12–15].

Our paper is devoted to the quantification of symmetry. Symmetry is conventionally described in a contrariety, binary manner, implying that the system is either completely symmetric or completely asymmetric. Fang et al. used the group theoretical approach to overcome this dichotomous problem and introduced the degree of symmetry as a non-negative continuous number ranging from zero to unity [16]. It was demonstrated that cross correlation sums are efficient for studying symmetries of strange attractors [17]. The method of so-called "detectives", based on the based on group-theoretic approach, was successfully implemented for the study of the symmetries of attractors in Refs. [18–20]. This deviation from the perfect geometric symmetry was quantified with as a "continuous measure of symmetry", introduced by Avnir, Zabrodsky, and co-workers in Refs. [21–25]. The continuous measure of symmetry in 1D shapes (lines) was defined as the minimal average square displacement of the points that a shape must undergo to attain the prescribed symmetry [21–25].

On the other hand, ordering in 2D patterns is usually quantified with Voronoi entropy, given by the following:

$$S_{vor} = -\sum_i P_i ln P_i, \quad (1)$$

where P_i is the portion of the polygons possessing n edges in a given Voronoi diagram (also called the coordination number of the polygon) and i is the total number of polygon types with a different number of edges [26–28]. In our recent papers, we demonstrated that the continuous measure of symmetry introduced in Refs. [24,25] and the Voronoi entropy of the given 2D pattern are not necessarily correlated [29,30]. Our previous paper is devoted to the alternative quantification of symmetry with the Shannon-like informational measure of symmetry, which was first introduced in Ref. [31], in which it was applied to the quantitative analysis of Voronoi diagrams arising from the Penrose tiling. In our present paper, we generalize and develop the notion of the informational measure of symmetry. An interpretation of the notion of the informational measure of symmetry follows the approach suggested in Ref. [32], namely, it is understood as an averaged uncertainty in the presence of symmetry elements from the group G in the given pattern [31,32]. We demonstrate that different approaches to the calculation of the informational measure of symmetry are possible.

2. Results and Discussion

2.1. Alternative Definitions of the Informational Measure of Symmetry

Consider a 2D pattern built of 1D and/or 2D shapes or lines, demonstrating a number of symmetry elements (rotational symmetry, centers of symmetry, axes of symmetry, etc.), denoted as G_i, $i = 1, 2 \ldots k$, where k is a number of non-identical symmetry operations. Pattern is understood as a 2D arrangement made from repeated lines or shapes on a surface. Element G_i forms the symmetry group of the shape G (which should be clearly distinguished from the symmetry group of the entire pattern). Thus, the informational measure of symmetry of the pattern (abbreviated to IMS) is defined in a Shannon-like form as follows:

$$H_{sym}(G) = -\sum_{i=1}^{k} P_i(G_i) ln P_i(G_i), \quad (2)$$

where $P_i(G_i)$ is the probability of appearance of the symmetry operation G_i within the shapes (lines) constituting the pattern, defined as follows:

$$P_i(G_i) = \frac{m(G_i)}{N_G} \leq 1, \quad (3)$$

where $N_G = \sum_{i=1}^{k} m(G_i)$ is the total number of symmetry elements (operations) appearing in the 1D or 2D shapes, recognized in a given pattern, and $m(G_i)$ is the number of the same symmetry elements (operations) G_i, calculated for a given pattern. The normalization condition given by Equation (4) takes place:

$$\sum_{i=1}^{k} P_i(G_i) = 1. \quad (4)$$

Let us explain in detail the meaning of the introduced Shannon measure of symmetry $H_{sym}(G)$. Suppose that we have a pattern demonstrating k distinguishable elements of symmetry with probability distribution $P_1(G_1) \ldots P_k(G_k)$. If, say, $P_i(G_i) = 1$, we are certain that an element of symmetry G_i is recognized within the shapes constituting the pattern; in other words, element G_i necessarily appears within all of the shapes constituting the pattern, and we are certain that it is present in the shapes. For any other value of $P_i(G_i)$, we are less certain about the occurrence of the symmetry element labeled i. Less certainty can be translated into more uncertainty [32]. Therefore, the larger the value of $-ln P_i(G_i)$, the larger the extent of uncertainty about the presence of element G_i within the pattern [32].

Multiplying $-lnP_i(G_i)$ by $P_i(G_i)$, and summing over all i, we obtain an average uncertainty about the presence of symmetry elements G_i within the given pattern. When $P_i(G_i) = 0$, we are certain that element G_i is not met within the pattern (numerous examples of calculation of $H_{sym}(G)$ are supplied below).

Alternatively, the symmetry of the pattern may be quantified with the parameter $\Omega_{sym}(G)$, defined according to Equation (5):

$$\Omega_{sym}(G) = -\sum_{n=1}^{l} P_n(n(G)) lnP_n(n(G)), \quad (5)$$

where n denotes the *total* number of elements of symmetry recognized in a shape; n changes from unity to the maximal number of elements of symmetry inherent for the shapes appearing in the pattern and denoted "l". $P_n(n(G))$ is the probability of finding the shape possessing n elements of symmetry in total belonging to group G within the pattern, defined as follows:

$$P_n(n(G)) = \frac{r(n(G))}{N_S}, \quad (6)$$

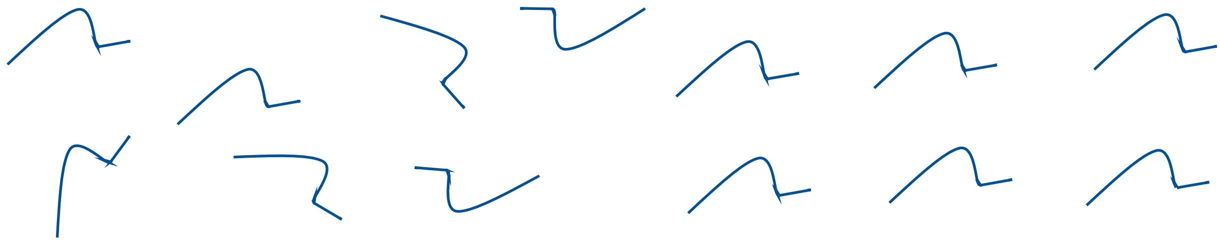
where $r(n(G))$ is the number of shapes possessing n elements of symmetry in total and N_S is the total number of shapes in the given pattern. The normalization condition given by Equation (7) takes place:

$$\sum_{n=1}^{l} P_n(n(G)) = 1 \quad (7)$$

The Shannon-shaped measure $\Omega_{sym}(G)$ is interpreted, in turn, as an average across the pattern uncertainty of finding the shape possessing in total n elements of symmetry within a given pattern [27,28]. The definition of the Shannon measure of symmetry $\Omega_{sym}(G)$ provided by Equations (5)–(7) resembles the definition of the Voronoi entropy, provided by Equation (1) with the following difference: instead of the number of polygon edges appearing in the definition of the Voronoi entropy, in our definition, we exploit the number of elements of symmetry n in the shape; thus, we label this measure as the Voronoi–Shannon measure of symmetry (VSMS). The definition of VSMS provided by Equations (5)–(7) latently implies that a more symmetrical shape is characterized by the larger number of symmetry elements. We illustrate the difference between the information-theoretic measure of symmetry (IMS) and the Voronoi–Shannon measure of symmetry with several examples. The paper is organized as follows: the measures of symmetry introduced by Equations (2)–(7) are calculated for the patterns built of (i) 1D shapes (curves); (ii) 2D shapes, namely triangles and ellipses; and (iii) mixed patterns comprised of 1D and 2D shapes.

2.2. Information-Theoretic Measures of Symmetry of the Patterns Built of 1D Objects

First, consider the IMS and the VSMS of the patterns comprising only 1D objects (lines) lying on a plane. It should be noted that the symmetry group of an object depends not only on the object itself but also on the space in which we view it. For example, the symmetry group of a line segment in R1 is of order 2, the symmetry group of a line segment considered as a set of points in R2 is of order 4, and the symmetry group of a line segments viewed as a set of points in R3 is of infinite order. Hereinafter, we assume that the considered objects (lines) are treated as sets of points in R2 space. Let us start from the pattern built of p irregular lines, such as depicted in Figure 1. The analysis should necessarily start from the establishment of the symmetry group of the pattern. In this case, we recognize that the single element of symmetry for the shapes constituting the pattern is the onefold rotational symmetry, reduced to the rotation of the lines by the angle $\varphi_1 = k\frac{2\pi}{1} = 2\pi$, denoted G_1, which is an identity element of the symmetry group.

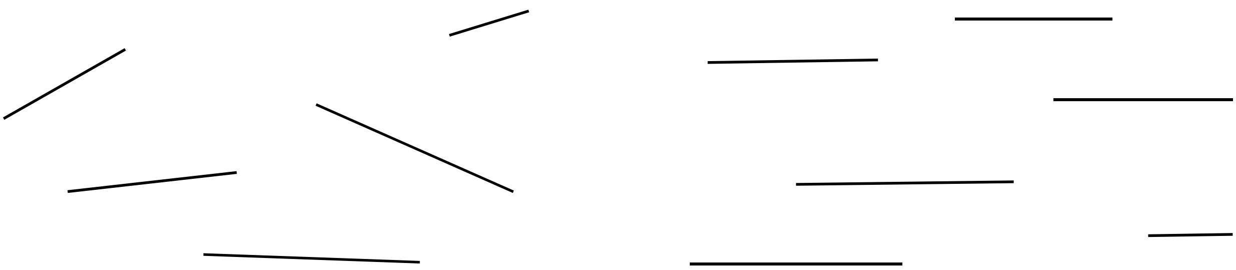


(**a**) $H_{sym}(G_1) = \Omega_{sym}(G_1) = 0$ (**b**) $H_{sym}(G_1) = \Omega_{sym}(G_1) = 0$

Figure 1. Pattern built of the 1D irregular (non-symmetrical) lines. (**a**) Random pattern; (**b**) regular pattern demonstrating the translational symmetry.

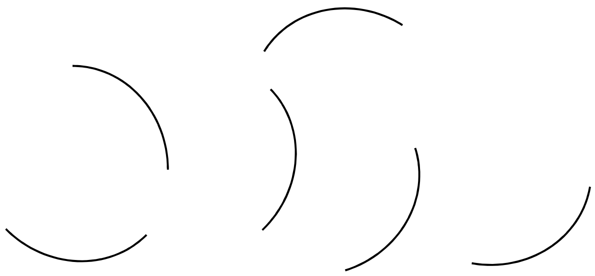
Let us first calculate H_{sym} for the pattern, shown in Figure 1a. In this case, $N_G = p$; thus, $P(G_1) = 1$, and consequently, we calculate $H_{sym}(G_1) = -P(G_1)lnP(G_1) = -1 \times ln1 = 0$. Now, we establish $\Omega_{sym}(G) = -\sum_{n=1}^{l} P_n(n(G))lnP_n(n(G))$. It is easily seen that, for the irregular shapes possessing a single element of symmetry, $P_n(n = 1) = 1$; hence, $\Omega_{sym}(G_1) = 0$. The same conclusion, i.e., $H_{sym}(G_1) = \Omega_{sym}(G_1) = 0$, holds for the pattern built from non-identical, irregular, non-symmetrical lines. It should be emphasized that the same conclusion., i.e., $H_{sym}(G_1) = \Omega_{sym}(G_1) = 0$, is true for the regular pattern, comprising irregular, non-symmetrical lines, such as the pattern shown in Figure 1b, demonstrating a pattern characterized by the translational symmetry. Thus, we concluded that both of the introduced measures of symmetry are insensitive to the long-range order. How should the obtained result be interpreted? $H_{sym}(G_1) = 0$ means that an averaged uncertainty to reveal symmetry operation G_1 within the pattern is zero; indeed, all of the 1D shapes depicted in Figure 1 possess this element of symmetry; in turn, $\Omega_{sym}(G_1) = 0$ means an average uncertainty for finding the shape demonstrating the single element of symmetry is zero within the pattern; indeed, every shape in the pattern has only one element of symmetry, namely G_1 (see Ref. [28]). It should be emphasized that neither Voronoi entropy nor continuous measure of symmetry could be defined and calculated for the patterns presented in Figure 1a,b.

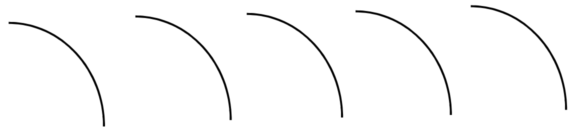
Now, consider the patterns composed of straight line segments, shown in Figure 2a,b, and seen as sets of points in R2 space. The symmetry group of the straight line segments is built of four elements, namely the unity element, which is the onefold rotational symmetry, which is the rotation by the angle $\varphi_1 = k\frac{2\pi}{1} = 2\pi$ (denoted G_1); the twofold rotational symmetry by the angle $\varphi_1 = k\frac{2\pi}{2} = \pi$, denoted G_2; and the mirror axes, denoted G_3 and G_4. Let us calculate H_{sym}. For the pattern, built of the p segments, we obtain $P(G_1) = P(G_2) = P(G_3) = P(G_4) = \frac{p}{4p} = \frac{1}{4}$; thus, $H_{sym} = -4\frac{1}{4}ln\frac{1}{4} = 1.39$.



(**a**) $H_{sym} = 1.39$, $\Omega_{sym} = 0.$ (**b**) $H_{sym} = 1.39$, $\Omega_{sym} = 0.$

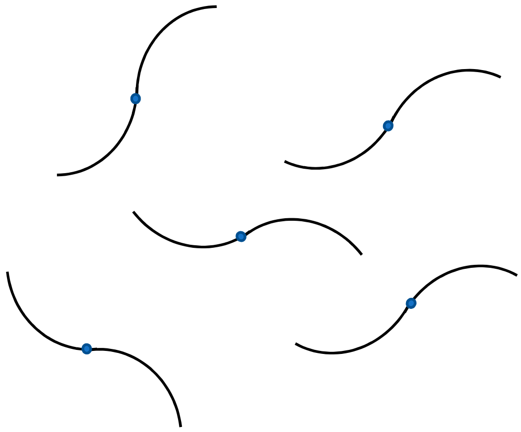
Figure 2. *Cont.*

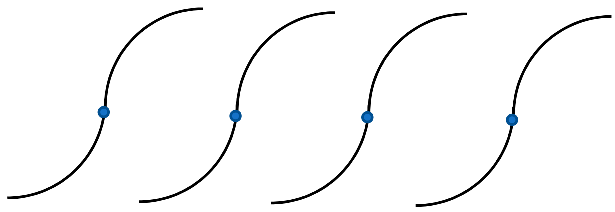




(**c**) $H_{sym} = 0.69, \ \Omega_{sym} = 0.$

(**d**) $H_{sym} = 0.69, \ \Omega_{sym} = 0.$





(**e**) $H_{sym} = 0.69, \ \Omega_{sym} = 0.$

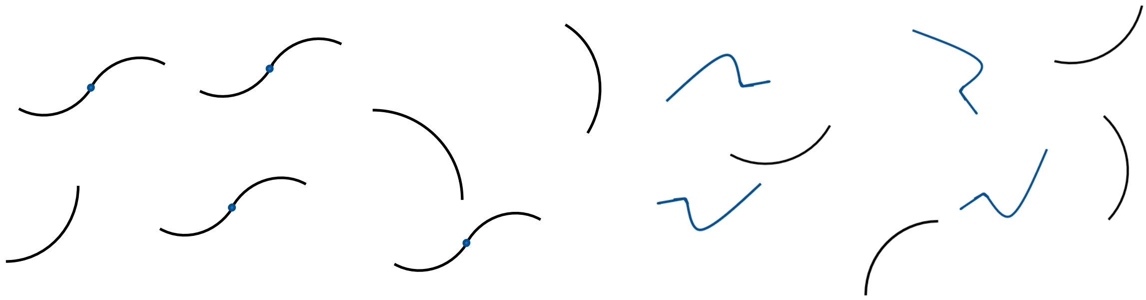
(**f**) $H_{sym} = 0.69, \ \Omega_{sym} = 0.$

Figure 2. Patterns built of shapes possessing two elements of symmetry: (**a**) random straight line segments, (**b**) ordered straight line segments, (**c**) random arcs of a circle, (**d**) ordered arcs of a circle, (**e**) random symmetrical segments of a cubic parabola, and (**f**) ordered symmetrical segments of a cubic parabola. The center of symmetry is shown by the blue circle.

Now, let us establish $\Omega_{sym}(G) = -\sum_{n=1}^{l} P_n(n(G)))lnP_n(n(G))$. In Figure 2a,b, all of the shapes in the patterns have four aforementioned elements of symmetry. Thus, $P_4(n = 4) = 1$, and hence, $\Omega_{sym} = 0$. Again, all of the measures of symmetry introduced coincide for the patterns presented in Figure 2a,b, and they are insensitive to the long-range order (translational symmetry) of segments, shown in Figure 2b.

Consider the patterns built of the p arcs of a circle (or, perhaps, the symmetric segments of the parabola $y = \alpha x^2$, $\alpha = const$, shown in Figure 2c,d. The symmetry group of the shapes depicted in Figure 2c,d is built of two elements, namely the unity element, which is the onefold rotational symmetry (denoted G_1), and the mirror axis, denoted G_2. For this kind of pattern, we obtain $(G_1) = P(G_2) = \frac{p}{2p} = \frac{1}{2}$; thus, $H_{sym} = -2\frac{1}{2}ln\frac{1}{2} = 0.69$. Consequently, in this case, $\Omega_{sym} = 0$ (due to $P_2(n = 2) = 1$ and $lnP_2 = 0$); the long-range order, shown in Figure 2d plays no role in the calculation of both measures of symmetry. Now, consider the patterns built of the p symmetric segments of a cubic parabola $y = \alpha x^3$, $\alpha = const$) shown in Figure 2e,f. The considerations akin to the aforementioned ones immediately yield $H_{sym} = 0.69$, $\Omega_{sym} = 0$. Thus, we come to the conclusion that the patterns depicted in Figure 2c–f are *equivalent* from the point of view of the Shannon measures of symmetry introduced, namely, H_{sym} and Ω_{sym}. Moreover, the VSMS of the patterns depicted in Figures 1 and 2 is equal; however, the IMS of the patterns shown in Figures 1 and 2 are different. It should be emphasized that both of the Shannon and the Voronoi–Shannon information-theoretic measures of symmetry of the discussed patterns are *the intensive properties* of the patterns and that they are independent of the area of the pattern or the density and size of the shapes, and in this sense, they are different from the true thermodynamic entropy, which is an extensive parameter of the system. It should be emphasized that the long-range order does not influence either of the information-theoretic measures of symmetry.

Consider now the mixed patterns, comprising 1D objects (lines), depicted in Figure 3.



(**a**) $H_{sym} = 1.03, \Omega_{sym} = 0.$ (**b**) $H_{sym} = 0.54, \Omega_{sym} = 0.69.$

Figure 3. Mixed patterns comprising 1D objects are depicted: (**a**) the pattern built from segments of cubic parabola and arcs of a circle, and (**b**) the pattern composed of irregular (non-symmetrical) shapes and arcs of a circle.

Let us start from the pattern comprising segments of a cubic parabola and arcs of a circle, shown in Figure 3a. Both shapes are characterized by the symmetry group containing two symmetry elements: the unity element, which is the onefold rotational symmetry and the twofold rotational symmetry in the case of segments of a cubic parabola, and the onefold rotational symmetry and the mirror axis in the case of arcs of a circle. Thus, $H_{sym} = 1.03$. Both shapes have two elements of symmetry; hence, $\Omega_{sym} = 0$. Now, consider the pattern built from p irregular, non-symmetrical curves and p arcs of a circle, presented in Figure 3b. We recognize two elements of symmetry in this pattern, namely the onefold rotational symmetry inherent for all of the shapes and denoted G_1, and the mirror axis labeled G_2 inherent for the arcs only. Thus, the entire number of the symmetry elements in the pattern is $N_G = 3p$ (see Equation (3)); consequently, we easily calculate $P(G_1) = \frac{2p}{3p} = \frac{2}{3}$; $P(G_2) = \frac{p}{3p} = \frac{1}{3}$; and finally, we obtain $H_{sym} = -\left(\frac{2}{3}ln\frac{2}{3} + \frac{1}{3}ln\frac{1}{3}\right) = 0.54$. Let us now calculate Ω_{sym} for the mixed pattern, shown in Figure 3b. For this pattern, we calculate ($N_s = 2p$): $P_1(n = 1) = \frac{p}{2p} = \frac{1}{2}$; $P_2(n = 2) = \frac{p}{2p} = \frac{1}{2}$; thus, $\Omega_{sym} = 0.69$. Again, the Voronoi entropy could not be introduced for the patterns presented in Figure 3a,b.

2.3. Information-Theoretic Measures of Symmetry of Patterns Built of 2D Shapes

Next, we address the patterns composed of 2D shapes. Let us start from the completely disordered pattern built of p irregular shapes depicted in Figure 4a. In this case, we recognize for all of the non-symmetrical shapes constituting the pattern the single element of symmetry, namely the rotation $\varphi_1 = k\frac{2\pi}{1} = 2\pi$; thus, $N_G = p$; $P(G_1) = 1$; and consequently, $H_{sym} = -\sum_{i=1}^{1} P(G_i)lnP(G_i) = -\sum_{i=1}^{1} 1ln(1) = 0$. It is easily seen that $\Omega_{sym}(G) = 0$ takes place for the same pattern. Let us analyze the 2D pattern comprising p identical equilateral triangles depicted in Figure 4b. The symmetry group of the equilateral triangle is the dihedral symmetry group, usually labeled D_3. In the case of the equilateral triangles shown in Figure 4b, we have $N_g = 6p$ elements of symmetry, which are $3p$ symmetry axes and $3p$ rotations. The IMS calculated with Equation (2) equals $H_{sym}(D_3) = 1.792$. On the other hand, all of the shapes constituting the pattern shown in Figure 4b have the same number of symmetry elements; thus, $\Omega_{sym}(D_3) = 0$.

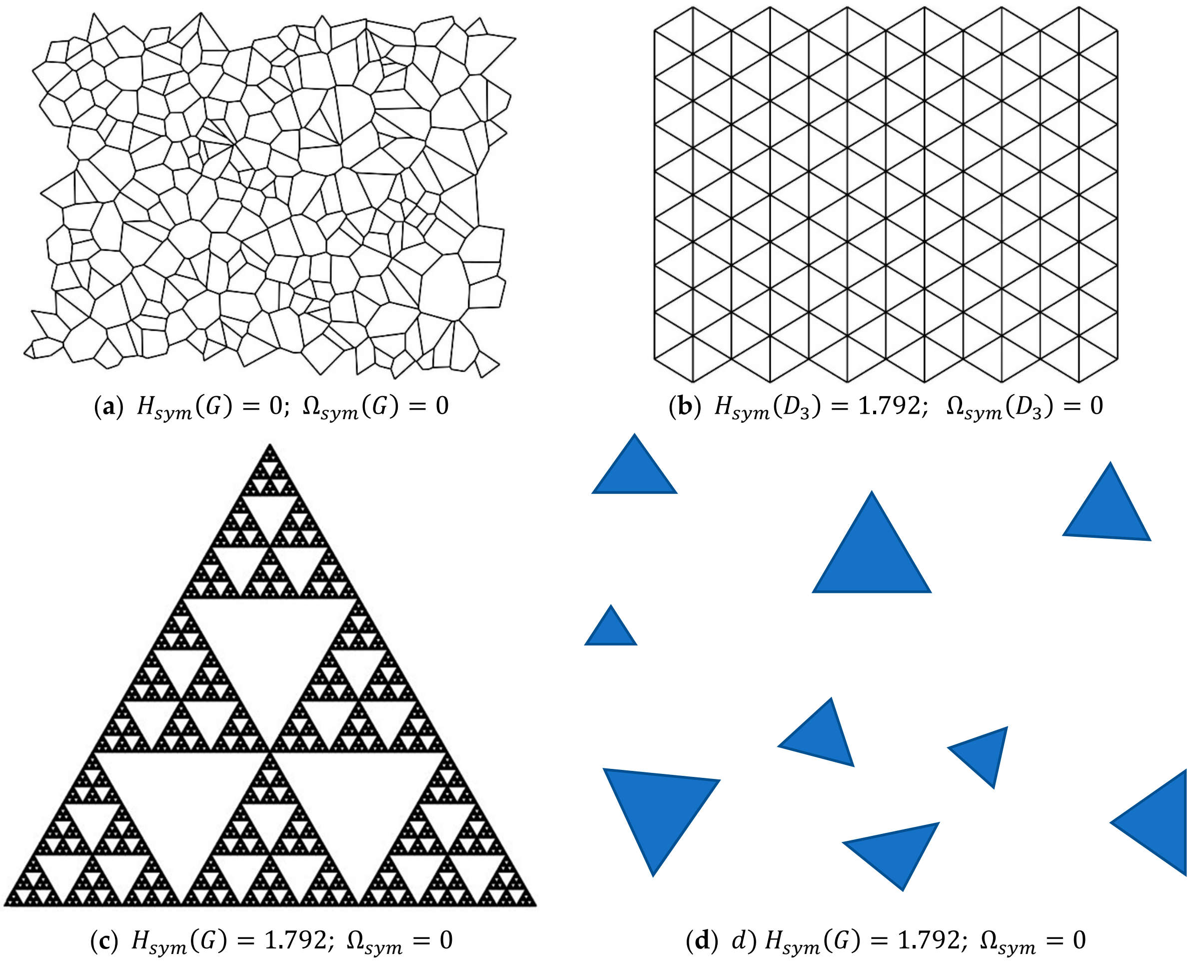


Figure 4. (**a**) Pattern filled with different unsymmetrical polygons, demonstrating $H_{sym}(G) = 0$; $\Omega_{sym}(G) = 0$. (**b**) Two-dimensional pattern comprising identical equilateral triangles, demonstrating $H_{sym}(G) = 1.792$; $\Omega_{sym} = 0$. (**c**) Sierpinski gasket built of equilateral triangles. (**d**) Pattern composed of the randomly dispersed equilateral triangles of various areas.

Consider the fractal Sierpinski gasket built of equilateral triangles, shown in Figure 4c [33,34]. It is easily seen that $H_{sym}(G) = 1.792$; $\Omega_{sym} = 0$ for any scaling level of its fractal structure. Thus, we conclude that informational measures of symmetry are invariant with respect to the scaling of the Sierpinski gasket. Obviously, the conclusion holds for the Sierpinski gasket built of squares. The general problem of the calculation of the informational measures of symmetry of fractal structures deserves additional research. The pattern characterized by the informational measures of symmetry should not be necessarily close-packed, as shown in Figure 4d, representing a set of randomly dispersed equilateral triangles of various areas. In this case, $H_{sym}(D_3) = 1.792$, $\Omega(D_3) = 0$ takes place. Again, the introduced informational measures of symmetry are insensitive to the presence/absence of the long-range order in a given pattern.

It is noteworthy that a pattern should not necessarily be built of polygons; it may comprise curvilinear shapes such as the ellipses, shown in Figure 5.

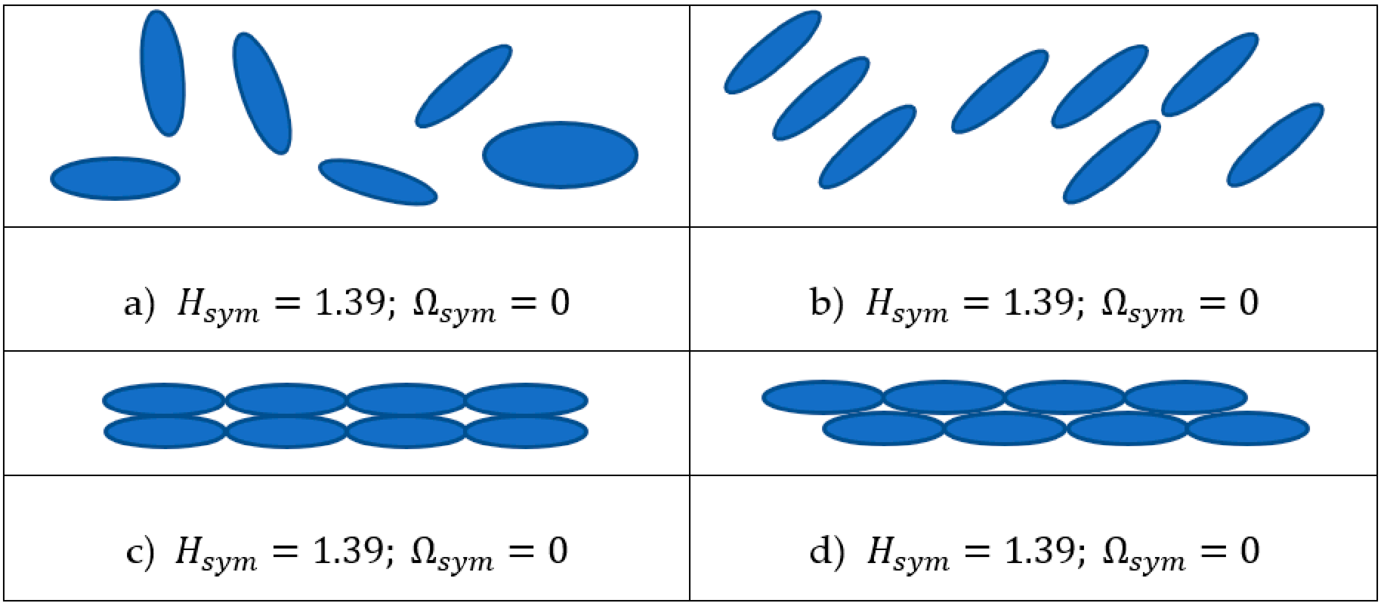


Figure 5. Patterns built from the ellipses are shown: (**a**) a pattern built of the dispersed random ellipses of various sizes; (**b**) a pattern built of dispersed ordered identical ellipses; (**c**) a pattern comprising close-packed identical ellipses, and the area between forms curvilinear quadrangles; (**d**) a pattern comprising close-packed identical ellipses, and the areas between form curvilinear triangles.

Let us start from the pattern depicted in Figure 5a comprising the dispersed random ellipses of various sizes. The group of symmetry of the ellipses includes four elements, namely the onefold rotational symmetry denoted G_1 , the twofold rotational symmetry denoted G_2 , and two distinguishable mirror axes denoted correspondingly as G_3 and G_4; in this case, $P(G_1) = P(G_2) = P(G_3) = P(G_4) = \frac{1}{4}$. Thus, we calculate $H_{sym} = -4\frac{1}{4}ln\frac{1}{4} = 1.39$. All of the ellipses have in total four elements of symmetry; hence, $\Omega_{sym} = 0$. The same is true for the dispersed identical long-range ordered ellipses, shown in Figure 5b. The same conclusion holds for the close-packed ordered identical ellipses forming the patterns shown in Figure 5c,d. Figure 5c,d illustrate the idea that the set of the shapes should be clearly defined. Indeed, $H_{sym} = 1.39$; $\Omega_{sym} = 0$ holds for the patterns built of the ellipses *only*. If we also consider the "interstitial" shapes emerging in the close-packed arranges (which are curvilinear quadrangles in Figure 5c and curvilinear triangles in Figure 5d), the informational measures of symmetry changes.

2.4. Information-Theoretic Measures of Symmetry of the Mixed Patterns Built of 2D and 1D Shapes

The suggested information measures of symmetry are easily generalized for the mixed patterns containing 1D and 2D shapes such as the pattern shown in Figure 6, which includes p irregular non-symmetric curves and p equilateral triangles.

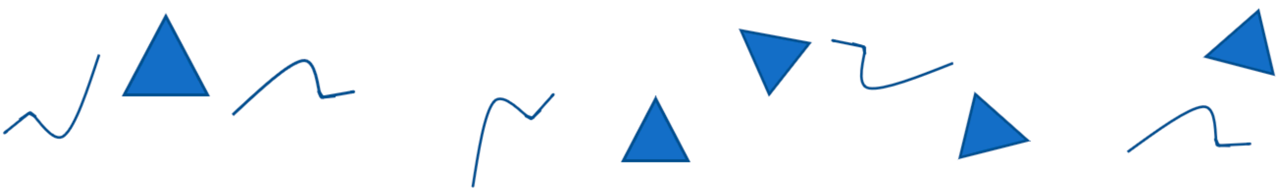


Figure 6. Mixed pattern built of p irregular non-symmetric curves and p equilateral triangles.

Let us quantify the symmetry of this pattern. The symmetry group of the equilateral triangle is the dihedral symmetry group D_3 containing $3p$ symmetry axes and $3p$ rotations (including the 2π rotation, denoted G_1). One more G_1 operation comes from the irregular curves; thus, we have in total $7p$ symmetry operations in this pattern. The IMS is easily calculated, according to $H_{sym} = -\left(\frac{2}{7}ln\frac{2}{7} + \frac{5}{7}ln\frac{1}{7}\right) = 2.23$. Now, we calculate VSMS of the same pattern; the probability of finding the shape possessing 6 elements of symmetry (triangles) in total within the pattern equals $\frac{1}{2}$, and the probability of finding the shape possessing a single element of symmetry (curves) within the pattern also equals $\frac{1}{2}$; thus, we obtain $\Omega_{sym} = -2 \times \frac{1}{2}ln\frac{1}{2} = 0.69$. Again, the Voronoi entropy and continuous measure of symmetry could not be reasonably introduced for the mixed pattern, depicted in Figure 6.

2.5. Information-Theoretic Measures of Symmetry as Dynamical Variables

Consider now N two-dimensional shapes (say ellipses and equilateral triangles shown in Figure 7) moving in a plane.

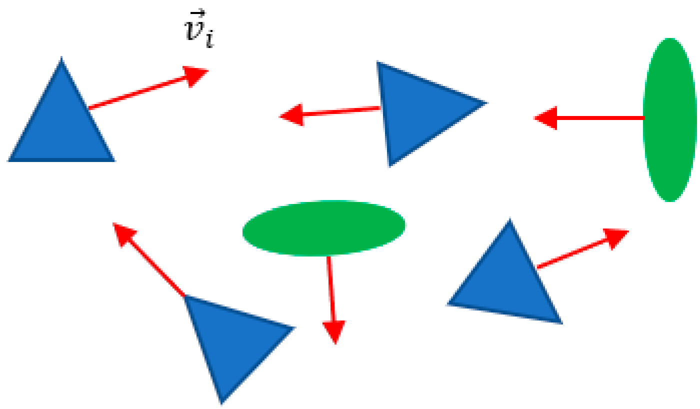


Figure 7. The planar movement of the ellipses and equilateral triangles is demonstrated. $\vec{v}_i$ is the velocity of the i-th shape.

The shapes (2D bodies) may collide elastically or stop their motion. If the symmetry of the bodies is conserved, we immediately conclude that the conservation laws $H_{sym} = const$; $\Omega_{sym} = const$ take place. Thus, in this case, conservation of the informational measures of symmetry also takes place. Consider now the less trivial situation depicted in Figure 8, where the p rhombi shown in Figure 8a "dissociate" with time into $2p$ equilateral triangles, shown in Figure 8b.

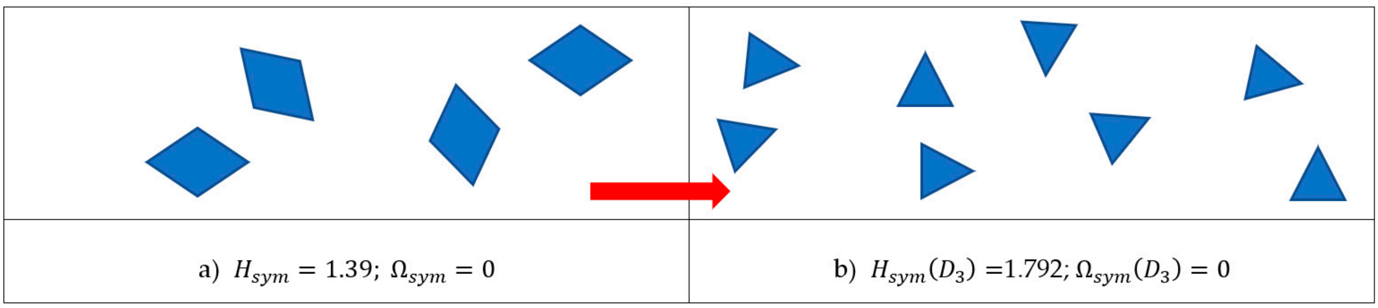


Figure 8. Time evolution of rhombi shown in (**a**), into equilateral triangles depicted in (**b**) is depicted.

The initial Shannon measures of the system of rhombi shown in Figure 8a coincide with that of the ellipses already calculated in Section 2.2, namely $H_{sym} = 1.39$; $\Omega_{sym} = 0$. After dissociation into equilateral triangles, we have $H_{sym}(D_3) = 1.792$; $\Omega_{sym}(D_3) = 0$ (see Section 2.2). This means that the change in the shape of the objects constituting the pattern is quite expectedly accompanied with a jump in the informational measure of symmetry accompanying the change in the symmetry group of the shapes. Hence, the information measure of symmetry introduced is well expected as useful for the characterization of phase transitions.

Last but not least, obviously the informational measures of symmetry could not be defined for the 0D objects (points). However, the set of points may be converted into the set of polygons with the use of the tessellation procedure prescribed (for example with the Voronoi tessellation [26–30]), and at the next stage, the informational measures of symmetry of the tessellations can be calculated.

2.6. Information-Theoretic Measures of Information: How Do They Work? An Example from Chemistry

Let us exemplify the information-theoretic measure information introduced with an example taken from chemistry. Consider the benzene combustion reaction, represented by Equation (8):

$$2C_6H_6 + 15O_2 \rightarrow\ 12CO_2 + 6H_2O \tag{8}$$

Figure 9 depicts the reaction schematically and demonstrates the elements of symmetry for the molecules involved. All of these molecules possess planar molecular geometry, which allows us to consider a reaction that takes place in R2 space. The molecule of benzene in the R2 space is characterized by twelve elements of symmetry, namely: $\frac{\pi}{3}$, $\frac{2\pi}{3}$, π, $\frac{4\pi}{3}$, $\frac{5\pi}{3}$, 2π rotations, and six mirror axes. The molecules of oxygen and CO_2 are linear ones and possess four elements of symmetry, namely π and 2π rotations, and two mirror axes. The molecule of water in R2 space possesses two elements of symmetry: 2π-rotation and the mirror axis, as shown inFigure 9.

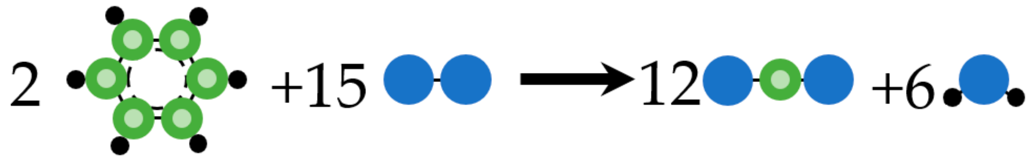


Figure 9. Combustion of benzene is depicted schematically: green circles depict atoms of carbon, black circles depict atoms of hydrogen, and blue circles depict atoms of oxygen.

Let us calculate how the chemical reaction changes the symmetry of the system. Our calculation conducted according Equations (2) and (5) demonstrates that, before the reaction, we obtain $H_{sym} = 2.01$; $\Omega_{sym} = 0.36$. $H_{sym} = 2.01$, which is due to the high symmetric benzene molecule, is as relatively high value. On the other hand, the value of $\Omega_{sym} = 0.36$ is relatively low. This means that a certain group of symmetry (namely group with the symmetry involving a linear molecule of oxygen) dominates in the system addressed before the reaction. This is easily understood; indeed, 15 molecules of oxygen react with two molecules of benzene. After the reaction, the value of H_{sym} decreases ($H_{sym} = 1.37$); this decrease is due to the diminished number of elements of symmetry inherent for the reaction products, namely water and CO_2 molecules. The value of Ω_{sym} is contrastingly increased, namely we established $\Omega_{sym} = 0.64$, which points to the more homogeneous distribution of the symmetry elements among products of the reaction. Thus, we conclude that the suggested measures of symmetry may be applied for quantification of the symmetry change occurring under chemical reactions.

3. Conclusions

This paper addresses the fine structures appearing in 2D patterns during the quantification of symmetry. The quantification of symmetry is a challenging task in biology (including understanding the structure of proteins [25] and the characterization of biological patterns [35]), physics (when applied for the characterization of attractors [18–20]), chemistry [23], and image processing [22]. Symmetry and ordering are usually quantified by the Voronoi entropy [26–30] and by the continuous measure of symmetry [21–25]. In this paper, we introduced and calculated the informational measures of various patterns built of 1D (curves) and 2D (shapes) objects. One of the Shannon-like measures of symmetry, labeled $H_{sym}(G)$, represents an average across the pattern uncertainty to find a symmetry operation related to the symmetry group G within the given pattern. The other Shannon-like measure of symmetry, $\Omega_{sym}(G)$, is interpreted as an averaged across the pattern uncertainty to find the shape possessing n elements of symmetry in total and forming the group G, which resembles the well-known Voronoi entropy [22–26,36]. We illustrated the measures of symmetry introduced with several patterns built of triangles, arcs, ellipses, rhombi, and irregular curves, including "mixed" patterns composed of 1D and 2D objects. The reported results strengthen the idea that the ordering and symmetry of a pattern can hardly be quantified with a single numerical value. We also calculated H_{sym} and Ω_{sym} for the Sierpinski fractal gasket built from equilateral triangles/squares. H_{sym} and Ω_{sym} remain the same for all scaling levels of the Sierpinski gasket [33,34]. The H_{sym} and Ω_{sym} introduced are the intensive parameters of the given pattern, and they are insensitive to the number of 1D/2D shapes, to their size, and to the area of the pattern. Both measures are influenced by the groups of symmetry of the shapes constituting the pattern. The time evolution of the Shannon measures of symmetry are considered. If the moving objects conserve their symmetry groups, the informational measures of symmetry are time independent. The time evolution of the Shannon measures of symmetry is illustrated with an example in which rhombi dissociate into equilateral triangles, thus changing the symmetry group of the pattern. A change in the suggested measures of symmetry under combustion of benzene is demonstrated. It is expected that the introduced Shannon measures of symmetry will be useful for the analysis of phase transitions. In future investigations, we plan to study (i) the informational measures of symmetry (IMS and VSMS) of fractals; (ii) the change in the informational measures of symmetry inherent in phase transitions; (iii) the IMS and VSMS of time crystals [37]; and (iv) the 3D generalization of Shannon-shaped measures introduced here.

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